Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Realizing non-close-packed crystal structures through directional binding of DNA-functionalized colloidal clusters TALID SINNO, MEHDI ZANJANI, JOHN CROCKER, Univ of Pennsylvania — A promising approach for engineering assembling entities that exhibit anisotropy is to create small clusters out of spherical colloidal particles. Here, we study computationally the self-assembly of large numbers of colloidal clusters formed by a recently-introduced crystal templating method. We study the assembly of clusters mediated by the addition of spherical 'bond' particles. In particular, the 'bond' spheres are DNA-functionalized so that they interact attractively with the clusters. In this construct, the differing number of particle-particle contacts available between a cluster and bond particle as a function of orientation creates directional bonding. A variety of simulation techniques are employed to study the thermodynamics and kinetics of the assembly process. Specifically, we compute nucleation barriers for several crystalline configurations using tetrahedral, octahedral, and cubic clusters. We show that some cluster types lead to facile growth of crystalline superstructures, while others lead to structures that are highly susceptible to defect formation. Crystal growth kinetics are probed using molecular dynamics and Brownian dynamics simulations and again demonstrate a wide range of kinetic limitations depending on the cluster geometry.

Talid Sinno
Univ of Pennsylvania

Date submitted: 11 Nov 2016 Electronic form version 1.4